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## Recent Advances in Unconventional Density Waves

Balázs Dóra

*The Abdus Salam ICTP, Strada Costiera 11, I-34014, Trieste, Italy*  
*dora@ictp.trieste.it*

Kazumi Maki

*Department of Physics and Astronomy, University of Southern California, Los Angeles CA*  
*90089-0484, USA*

Attila Virosztek

*Department of Physics, Budapest University of Technology and Economics, H-1521 Budapest,*  
*Hungary and Research Institute for Solid State Physics and Optics, P.O.Box 49, H-1525*  
*Budapest, Hungary*

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Unconventional density wave (UDW) has been speculated as a possible electronic ground state in excitonic insulator in 1968. Recent surge of interest in UDW is partly due to the proposal that the pseudogap phase in high  $T_c$  cuprate superconductors is d-wave density wave (d-DW).

Here we review our recent works on UDW within the framework of mean field theory. In particular we have shown that many properties of the low temperature phase (LTP) in  $\alpha$ -(BEDT-TTF)<sub>2</sub>MHg(SCN)<sub>4</sub> with M=K, Rb and Tl are well characterized in terms of unconventional charge density wave (UCDW). In this identification the Landau quantization of the quasiparticle motion in a magnetic field (the Nersesyan effect) plays the crucial role. Indeed the angular dependent magnetoresistance and the negative giant Nernst effect are two hallmarks of UDW.

### 1. Introduction

Until recently the electronic ground states in crystalline solids are considered to belong to one of four canonical ground states in quasi-one dimensional systems: s-wave superconductors, p-wave superconductors, (conventional) charge density wave and (conventional) spin density wave [1–3]. Indeed many systems discovered since 1972 appeared to accommodate in this scheme: CDW in NbSe<sub>3</sub> and SDW in Bechgaard salts (TMTSF)<sub>2</sub>PF<sub>6</sub> [4]. In all of these systems the quasiparticle spectrum has the energy gap  $\Delta$  and the quasiparticle density decreases exponentially as  $e^{-\Delta/T}$  as the temperature decreases to  $T \ll \Delta$ . Also the thermodynamics of these systems are practically the same as the one for s-wave superconductors as described by the theory of Bardeen, Cooper and Schrieffer [5] (i.e. the BCS theory).

However since the discovery of heavy fermion superconductors, organic superconductors, high  $T_c$  cuprate superconductors and  $\text{Sr}_2\text{RuO}_4$ , this simple picture has to be necessarily modified. First of all most of these new superconductors are unconventional and nodal [6–8]. For more recent developments on this subject the reader may consult Ref. [9].

Parallel to this development, intense research has been done during the past few years in order to explore the properties of density wave with order parameter  $\Delta(\mathbf{k})$ , which depends on the quasiparticle momentum along the Fermi surface. We call these states unconventional density waves (UDW) in parallel to unconventional superconductivity.

This kind of condensates was first speculated on by Halperin and Rice [10] as a possible ground state in the excitonic insulator. However unlike conventional density waves, there will be no x-ray signal or spin signal associated with UDW since the average of  $\Delta(\mathbf{k})$  over the Fermi surface usually vanishes (i.e.  $\langle \Delta(\mathbf{k}) \rangle = 0$ ).

Therefore one may think that UDW has a truly quantum mechanical order parameter somewhat similar to superconductors. UDW is not accompanied by the spatial variation of charge or spin. This intriguing property is known as hidden-order in recent literature [11]. In order to make the hidden order visible, we need impurities for example [12]. Also unlike conventional density waves the nodal excitations persist to  $T = 0$  K, giving rise to electronic specific heat  $\sim T^2$ , where  $T$  is temperature. Indeed the thermodynamics is practically the same as the one for d-wave superconductors [13, 14]. The recent surge in UDW is generated by the possibility that the pseudogap phase in high  $T_c$  cuprates is d-wave density wave (d-DW) [11, 15, 16]. The angle resolved photoemission spectra (ARPES) in the pseudogap phase indicate that the energy gap  $\Delta(\mathbf{k})$  is the same as in d-wave superconductors [17]. Further the mysterious relation  $\Delta(0) = 2.14T^*$  found in LSCO, YBCO and Bi2212 [18–20] can be readily interpreted in terms of d-DW. Here  $\Delta(0)$  is the maximum value of the energy gap determined by STM and  $T^*$  is the pseudogap temperature which is identified with the transition to d-DW. Actually 2.14 is the weak-coupling value for the d-wave superconductors.

The nature of the low-temperature phase (LTP) in quasi-two dimensional organic conductors  $\alpha\text{-(BEDT-TTF)}_2\text{MHg(SCN)}_4$  with  $M=\text{K, Rb and Tl}$  has not been understood until recently [21]. Although the phase transition is clearly seen in magnetotransport measurements, neither charge, nor magnetic order has been established [22, 23]. Moreover the destruction of this LTP in an applied magnetic field suggests a kind of CDW rather than SDW. On the other hand the temperature dependence of the threshold electric field associated with the sliding motion of DW [24] is very different from the one in typical CDW but somewhat similar to the one in SDW [25]. In fact, we have succeeded in describing the temperature dependence of the threshold electric field in terms of UCDW with imperfect nesting [26, 27].

However, the LTP of  $\alpha\text{-(BEDT-TTF)}_2\text{KHg(SCN)}_4$  is also well-known for its striking angular dependent magnetoresistance (ADMR) [28–31]. There have been many attempts to interpret this phenomenon in terms of the reconstructed Fermi

surface. Rather we find that the Landau quantization of the quasiparticle orbit in UDW as described by Nersesyan et al. [32, 33] plays the crucial role here [34, 35]. More recently we find that the same Landau quantization gives rise to large negative Nernst effect in UDW [36]. Indeed we can describe the large Nernst effect observed in  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub> [37] in terms of UCDW. Therefore we may conclude that the LTP in  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub> with M=K, Rb and Tl is UCDW. Also the LTP in  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub> below  $T_c = 135$  K share many features common to UCDW [38]. We shall discuss this briefly in Section 2.

The possibility of UCDW in 2H-NbSe<sub>2</sub> and USDW in the antiferromagnetic phase in URu<sub>2</sub>Si<sub>2</sub> have also been suggested [39, 40]. We believe that the large negative Nernst effect observed in 2H-NbSe<sub>2</sub> [41] and the micromagnetism seen in URu<sub>2</sub>Si<sub>2</sub> [12, 42] appeared to have confirmed UCDW in the former, USDW in the latter. As has already been mentioned, the pseudogap phase in high  $T_c$  cuprates is most likely d-DW, though we prefer d-SDW to d-CDW [16].

In the following we shall first summarize the quasiparticle spectrum, the thermodynamics and other properties of UDW in Section 2. Then in Section 3.-5., we discuss the Nersesyan effect for UDW in a magnetic field. This important work appears to be neglected by most people working on UDW. In particular the striking ADMR and the large negative Nernst signal immediately follow from the Nersesyan effect. Therefore in particular the giant Nernst effect is the hallmark of UDW. We believe, that the large Nernst signal observed in underdoped LSCO, YBCO and Bi2212 indicates clearly that they are UDW [43–46].

In Section 6. we speculate the likely places where one can find UDW. Still very few UDW's have been identified. Therefore the field of UDW is still widely open and UDW will be found in unexpected places.

## 2. BCS theory of unconventional density waves

In the following we shall consider quasi-one or quasi-two dimensional systems, with the Hamiltonian given by

$$H = \sum_{\mathbf{k}, \sigma} \xi(\mathbf{k}) a_{\mathbf{k}, \sigma}^+ a_{\mathbf{k}, \sigma} + \frac{1}{2} \sum_{\substack{\mathbf{k}, \mathbf{k}', \mathbf{q} \\ \sigma, \sigma'}} V(\mathbf{k}, \mathbf{k}', \mathbf{q}) a_{\mathbf{k}+\mathbf{q}, \sigma}^+ a_{\mathbf{k}, \sigma} a_{\mathbf{k}'-\mathbf{q}, \sigma'}^+ a_{\mathbf{k}', \sigma'}, \quad (1)$$

where  $a_{\mathbf{k}, \sigma}^+$  and  $a_{\mathbf{k}, \sigma}$  are the creation and annihilation operators of electrons with momentum  $\mathbf{k}$  and spin  $\sigma$ ,  $\xi(\mathbf{k})$  is the kinetic energy of electrons measured from the Fermi energy in the normal state and  $V(\mathbf{k}, \mathbf{k}', \mathbf{q})$  is the interaction between particles. In the following we shall approximate it as

$$V(\mathbf{k}, \mathbf{k}', \mathbf{q}) = 2V f(\mathbf{k}) f(\mathbf{k}') \delta(\mathbf{q} - \mathbf{Q}), \quad (2)$$

where  $\mathbf{Q}$  is the nesting vector. Also for simplicity we limit ourselves to UCDW though a parallel treatment of USDW is possible. Then within the mean field ap-

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proximation Eq. (1) is recasted as

$$H = \sum_{\mathbf{k}, \sigma} \left( \xi(\mathbf{k}) a_{\mathbf{k}, \sigma}^+ a_{\mathbf{k}, \sigma} + \Delta(\mathbf{k}) a_{\mathbf{k}, \sigma}^+ a_{\mathbf{k}+\mathbf{Q}, \sigma} + \bar{\Delta}(\mathbf{k}) a_{\mathbf{k}+\mathbf{Q}, \sigma}^+ a_{\mathbf{k}, \sigma} \right) - \sum_{\mathbf{k}} \frac{|\Delta(\mathbf{k})|^2}{V \langle |f(\mathbf{k})|^2 \rangle} \quad (3)$$

and

$$\Delta(\mathbf{k}) = V f(\mathbf{k}) \sum_{\mathbf{k}', \sigma} f(\mathbf{k}') \langle a_{\mathbf{k}'-\mathbf{Q}, \sigma}^+ a_{\mathbf{k}', \sigma} \rangle. \quad (4)$$

This is expressed in terms of Nambu's spinor [47] as

$$H = \sum_{\mathbf{k}, \sigma} \Psi_{\sigma}^+(\mathbf{k}) \left( \tilde{\xi}(\mathbf{k}) \rho_3 + \eta(\mathbf{k}) + \Delta(\mathbf{k}) \rho_1 \right) \Psi_{\sigma}(\mathbf{k}), \quad (5)$$

where  $\tilde{\xi}(\mathbf{k}) = (\xi(\mathbf{k}) - \xi(\mathbf{k} - \mathbf{Q}))/2$  and  $\eta(\mathbf{k}) = (\xi(\mathbf{k}) + \xi(\mathbf{k} - \mathbf{Q}))/2$ . In the following we shall take the tilde off from  $\xi$ . The Green's function is then given by

$$G^{-1}(\omega, \mathbf{k}) = \omega - \xi(\mathbf{k}) \rho_3 - \eta(\mathbf{k}) - \Delta(\mathbf{k}) \rho_1. \quad (6)$$

The pole of  $G(\omega, \mathbf{k})$  gives the quasiparticle spectrum as

$$\omega = \eta(\mathbf{k}) \pm \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2} \quad (7)$$

In most of quasi-one or quasi-two dimensional systems  $\xi(\mathbf{k})$  depends only on  $\mathbf{k}$  perpendicular to the Fermi surface. So we can write  $\xi(\mathbf{k}) = v(k_a - k_F)$ , where  $v$  is the Fermi velocity. Then in many cases we can take  $\Delta(\mathbf{k}) = \Delta f(\mathbf{k})$  with  $f(\mathbf{k}) = \sin(bk_b)$  or  $\cos(bk_b)$ . Further if we can neglect  $\eta(\mathbf{k})$ , the imperfect nesting term, the quasiparticle density of states is obtained as [13]

$$\frac{N(E)}{N_0} = \text{Re}|E| \left\langle \frac{1}{\sqrt{E^2 - \Delta(\mathbf{k})^2}} \right\rangle = \begin{cases} \frac{2}{\pi} x K(x) & \text{for } x < 1 \\ \frac{2}{\pi} K(x^{-1}) & \text{for } x > 1 \end{cases}, \quad (8)$$

where  $x = |E|/\Delta$  and  $K(x)$  is the complete elliptic integral of the first kind. The quasiparticle density of states is shown in Fig. 1.

Also the thermodynamics is similarly obtained [48–50]. For this purpose it is necessary to solve the gap equation

$$\lambda^{-1} = \langle f^2 \rangle^{-1} \int_0^{v k_F} dE \text{Re} \left\langle \frac{f^2}{\sqrt{E^2 - \Delta^2 f^2}} \right\rangle \tanh \frac{E}{2T}. \quad (9)$$

Here we have neglected the imperfect nesting term for simplicity. The gap equation is the same as for d-wave superconductors. We obtain  $\Delta(0)/T_c = 2.14$  and

$$\frac{\Delta(T)}{\Delta(0)} \cong \sqrt{1 - \left( \frac{T}{T_c} \right)^3}. \quad (10)$$

In Fig. 2 the exact solution of  $\Delta(T)$  [13] with the approximate one is shown. Therefore Eq. (10) is very useful for semiquantitative analysis. In very clean systems

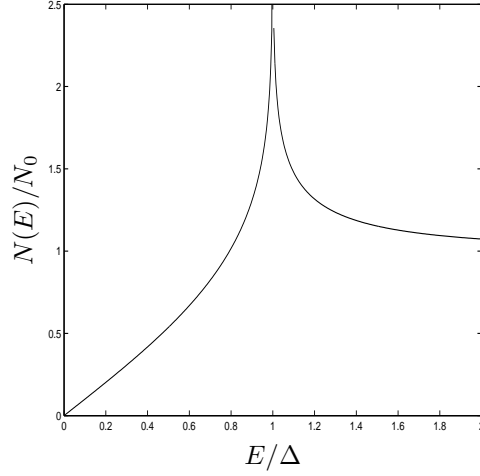
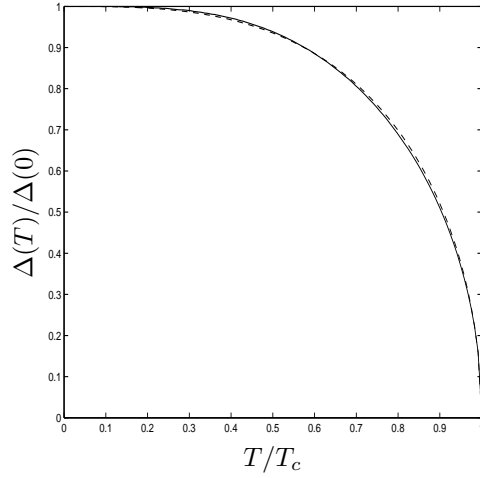


Fig. 1. The quasiparticle density of states of UDW is shown.

Fig. 2. The order parameter  $\Delta(T)$  is shown (solid line) together with the approximate solution Eq. (10) (dashed line).

when the quasiparticle scattering is limited by impurity scattering, the electric conductivity is well approximated by

$$\frac{\sigma(T)}{\sigma_n} = \frac{4}{\pi} \int_0^{\pi/2} d\phi (1 + \exp \beta \Delta \sin \phi)^{-1} \simeq \begin{cases} 1 - \beta \Delta / \pi & \text{for } T \simeq T_c \\ \frac{4}{\pi} \ln(2) (\beta \Delta)^{-1} & \text{for } T \ll T_c \end{cases} \quad (11)$$

Unfortunately this  $T$  linear behaviour for small temperatures cannot describe the  $T^3$  dependence of the electric conductivity of  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub> [38]. This suggests rather that the electric current  $\mathbf{J} \parallel \mathbf{b}$  is perpendicular to the nodal lines of

UCDW. In other words this implies  $\Delta(\mathbf{k}) = \Delta \sin(bk_b)$  in  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub>. This is somewhat surprising, since in  $\alpha$ -(BEDT-TTF)<sub>2</sub>MHg(SCN)<sub>4</sub>, what we are going to describe in some details, we found  $\Delta(\mathbf{k}) = \Delta \sin(ck_c)$  [34, 35]. In the present configuration, we obtain

$$\frac{\sigma_b(T)}{\sigma_{bn}} = \frac{8}{\pi} \int_0^{\pi/2} d\phi \sin(\phi)^2 (1 + \exp \beta \Delta \sin \phi)^{-1} \simeq \begin{cases} 1 - \beta \Delta / 3\pi & \text{for } T \simeq T_c \\ \frac{12}{\pi} \zeta(3) (\beta \Delta)^{-3} & \text{for } T \ll T_c \end{cases} \quad (12)$$

Especially for  $T < T_c/2$ ,  $\sigma_b(T) \sim T^3$ , in accordance with the experimental data from  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub>.

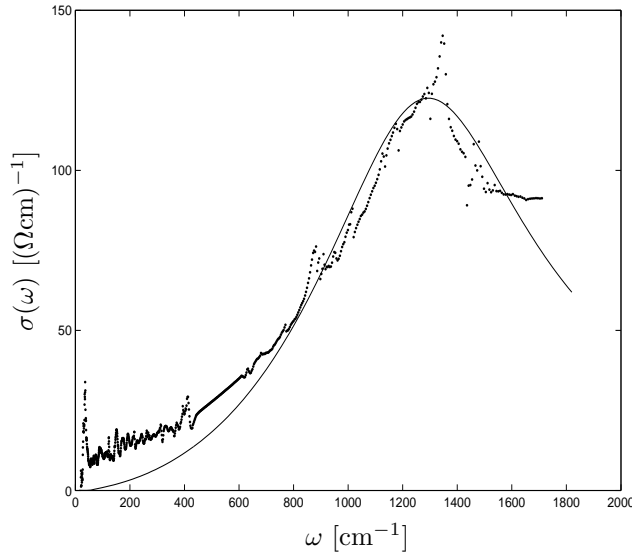


Fig. 3. The optical conductivity of  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub> at  $T = 60$  K [38] is plotted together with our theoretical prediction.

We show the optical conductivity with small impurity scattering rate in the Born limit [51, 52], and the result is compared to the optical data taken at  $T = 60$  K in Fig. (3). We think that the agreement is excellent. Also from this figure we can extract  $\Delta \simeq 930$  K, which is about 3 times larger than the one expected from the weak-coupling theory  $2.14 \times 135 \cong 290$  K. In conventional CDW and SDW, such a large deviation from the weak coupling theory result is mostly ascribed to the imperfect nesting term [53, 54].

Therefore the transition in UDW is metal to metal. In general the conductivity in UDW is anisotropic reflecting the direction of  $\mathbf{J}$  relative to the direction of the nodal lines. For example we believe that the  $T$  linear resistivity in the pseudogap phase in high  $T_c$  cuprates and heavy fermion systems are in part due to UDW. In these systems, the normal state resistance is proportional to  $T^2$  as in the Landau

Fermi liquid theory [55–57]. In these systems, the quasiparticle lifetime is dominated by electron-electron scattering. Then in UDW this  $T^2$  behaviour changes into  $T$  linear resistance as is readily seen from Eq. (11). This behaviour is often called "non Fermi liquid". But we think that this word is very misleading and should only be used with care. Actually the quasiparticle in UDW is bona fide Fermi particle. In the spirit of Landau, the Fermi liquid has to be defined as the Fermion, which has charge  $\pm e$  and spin  $1/2$  and is described by a pole of Green's function as given in Eq. (6). In this case, we can describe both the thermodynamics and transport properties of the system in terms of standard many body technique as in the book of Abrikosov, Gor'kov and Dzyaloshinskii [58].

### 3. The Nersesyan effect

This surprising effect of the magnetic field on the quasiparticle spectrum in UDW was first discussed in Ref. [32, 33]. The quasiparticle spectrum in the presence of magnetic field is obtained from

$$(E - \xi(\mathbf{k} + e\mathbf{A})\rho_3 - \eta(\mathbf{k} + e\mathbf{A}) - \Delta(\mathbf{k} + e\mathbf{A})\rho_1)\Psi(\mathbf{r}) = 0, \quad (13)$$

where we have introduced the magnetic field through the vector potential  $\mathbf{A}$ . It is readily recognized that Eq. (13) has the same mathematical structure as the Dirac equation in a magnetic field studied in 1936 [59, 60]. For simplicity let us assume that the Fermi surface is parallel to the  $a - c$  plane and the  $b$  direction is perpendicular to the  $a - c$  plane. Also  $\xi(\mathbf{k})$  depends only on  $k_a$  while  $\Delta(\mathbf{k})$  only on  $k_c$ . Also for a while we neglect  $\eta(\mathbf{k})$  since in many cases  $\eta(\mathbf{k}) \ll \max |\Delta(\mathbf{k})|$ . Then the quasiparticle energy spectrum depends only on the magnetic field component parallel to  $b$ . It is more convenient to rewrite Eq. (13) as [36]

$$E\Psi = (-iv_a\partial_x\rho_3 + \Delta ceBx\cos(\theta)\rho_1)\Psi, \quad (14)$$

$\theta$  is the angle the magnetic field makes with the  $b$  axis. We find

$$E^2 = 2nv_a\Delta ce|B\cos\theta|, \quad (15)$$

where  $n = 0, 1, 2, \dots$ . The Landau wavefunctions are given by

$$\Psi_0 = \begin{pmatrix} i \\ 1 \end{pmatrix} \phi_0, \quad (16)$$

$$\Psi_{n \neq 0} = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 \\ i \end{pmatrix} \phi_{n-1} \pm \begin{pmatrix} i \\ 1 \end{pmatrix} \phi_n \right], \quad (17)$$

where  $\phi_n$  is the  $n$ -th wavefunction of a linear harmonic oscillator with parameters "mass"  $m = 1/2v_a^2$  and "frequency"  $\omega = 2v_a\Delta ceB\cos(\theta)$ . From Eq. (17) it is obvious, that the  $n \neq 0$  levels are twofold degenerate, since  $\Psi_{n \neq 0}$  is composed of the  $n - 1$ -th and  $n$ -th wavefunction of the harmonic oscillator.

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So far we have neglected the imperfect nesting term. To be concrete, we assume that

$$\eta(\mathbf{k}) = \sum_{n=-\infty}^{\infty} \varepsilon_n \cos(2\mathbf{d}_n \mathbf{k}), \quad (18)$$

where  $\mathbf{d}_n$ 's are selected lattice vectors. In the LTP of  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>, the multidip structure of the angular dependent magnetoresistance (ADMR) is accounted for by similar  $\eta(\mathbf{k})$  [35]. Then the imperfect nesting term removes the degeneracy of  $E_{n \neq 0}$  and the Landau levels become

$$E_{0,1} = -E_0^{(1)}, \quad (19)$$

$$E_{1,1} = \pm E_1 - E_1^{(1)}, \quad (20)$$

$$E_{1,2} = \pm E_1 - E_1^{(2)}, \quad (21)$$

and

$$E_n = \sqrt{2nv_a \Delta c e B |\cos(\theta)|}, \quad (22)$$

$$E_0^{(1)} = E_1^{(1)} = \sum_m \varepsilon_m \exp(-y_m), \quad (23)$$

$$E_1^{(2)} = \sum_m \varepsilon_m (1 - 2y_m) \exp(-y_m), \quad (24)$$

and  $y_m = v_a b^2 e |B \cos(\theta)| (\tan(\theta) \cos(\phi - \phi_o) - \tan(\theta_m))^2 / \Delta c$ ,  $\tan \theta_0 \simeq 0.5$ ,  $d_0 \simeq 1.25$ ,  $\phi_0 \simeq 27^\circ$ . Here  $\phi$  is the angle the projected magnetic field on the  $a$ - $c$  plane makes with the  $c$ -axis.

With the help of the quasiparticle spectrum, the thermodynamic properties are readily determined as done in Ref. [32, 33]. In the following we shall consider the ADMR and the magnetothermopower.

#### 4. Angular dependent magnetoresistance (ADMR)

In the low temperature and high field limit (i.e.  $\beta E_1 \gg 1$ , where  $\beta = 1/T$ ), we assume that the quasiparticle transport is dominated by the  $n = 0$  and  $n = 1$  Landau levels. Also for concreteness let us consider the magnetoresistance in the LTP of  $\alpha$ -(BEDT-TTF)<sub>2</sub>MHg(SCN)<sub>4</sub> with M=K, Rb and Tl [35]. The Fermi surface of this system is sketched in Fig. 4 together with the related field configuration.

As is readily seen from Fig. 4, the Fermi surface in  $\alpha$ -(BEDT-TTF)<sub>2</sub>MHg(SCN)<sub>4</sub> salts consists of quasi-one dimensional sheets and quasi-two dimensional ellipses. Further we assume that UCDW appears only on the quasi-one dimensional sheets while the one with the quasi-two dimensional Fermi surface remains in the normal state. Then within the two level approximation, the magnetoresistance is given by

$$R(B, \theta, \phi)^{-1} = 2\sigma_1 \left( \frac{\exp(-x_1) + \cosh(\zeta_0)}{\cosh(x_1) + \cosh(\zeta_0)} + \frac{\exp(-x_1) + \cosh(\zeta_1)}{\cosh(x_1) + \cosh(\zeta_1)} \right) + \sigma_2, \quad (25)$$



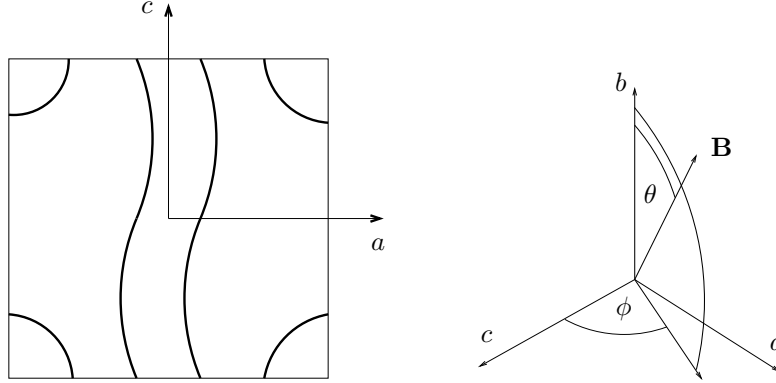


Fig. 4. The Fermi surface of  $\alpha$ -(BEDT-TTF) $_2$ K(HgSCN) $_4$  is shown in the left panel. In the right one the geometrical configuration of the magnetic field with respect to the conducting plane is plotted.

where  $x_1 = \beta E_1$ ,  $\zeta_0 = \beta E_1^{(1)}$ ,  $\zeta_1 = \beta E_1^{(2)}$ . Here  $\sigma_1$  and  $\sigma_2$  are the conductivities associated with the  $n = 1$  Landau level and the  $n = 0$  level plus the contribution from the elliptical Fermi surface, respectively. First let us consider the case when  $B$  is normal to the conducting plane ( $\theta = 0$ ). In the present configuration, the imperfect nesting plays no role and we can set  $\zeta_0 = \zeta_1 = 0$ .

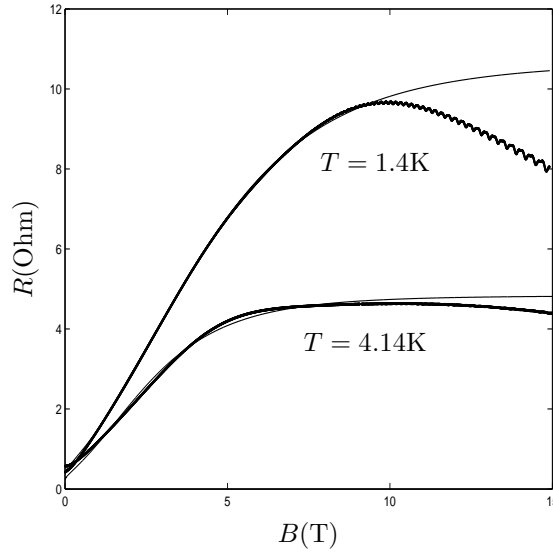


Fig. 5. The magnetoresistance is plotted for  $T = 1.4\text{K}$  and  $4.14\text{K}$  as a function of magnetic field. The thick solid is the experimental data, the thin one denotes our fit based on Eq. (25).

In Fig. 5 we show the  $B$  dependence of the magnetoresistance of single crystal

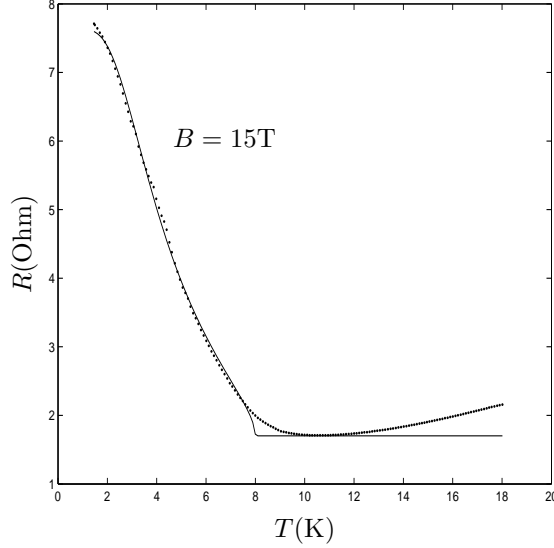


Fig. 6. The temperature dependent magnetoresistance is shown at  $B = 15$  T. The dots are the experimental data, the solid line is our fit.

of  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub> for  $T = 1.4$  K and  $T = 4.14$  K. As seen in Fig. 5, the fitting improves further as the temperature decreases, though a clear deviation from the otherwise excellent fitting starts around  $B = 8$  T. This can come from the Landau quantization of the quasi-two dimensional Fermi surface, what we ignored so far. In Fig. 6, we show the temperature dependence of the magnetoresistance for  $B = 15$  T. The fitting is almost perfect down to  $T \simeq 2$  K. The deviation around  $T = 8$  K is clearly due to the fact that we have to include more Landau levels as  $T$  approaches  $T_c$ . From these fittings we can extract  $\sigma_2/\sigma_1 \sim 0.1$  and  $0.3$ ,  $\Delta(0) = 17$  K (the corresponding weak-coupling value),  $v \sim 6 \times 10^6$  cm/s. Also we have used Eq. (10) for  $\Delta(T)$ .

In Figs. 7 and 8, we show the ADMR data taken at  $T = 1.4$  K,  $B = 15$  T and  $\phi = 45^\circ$ . As is readily seen, the fittings are excellent. From this we deduce  $\sigma_2/\sigma_1 \sim 0.1$ ,  $b \sim 30$  Å,  $\varepsilon_0 \sim 3$  K. This  $b$  is comparable to the lattice constant  $b = 20.26$  Å. Finally in Fig. 9 we show  $R$  versus  $\theta$  for different  $\phi$  and compare to the experimental data side by side. Perhaps there are still differences in some details, but the overall agreement is very striking. The present model can describe a similar figure found in Ref. [31] as well. In summary, the Landau quantization of the quasiparticle spectrum in UDW as shown by Nersesyan et al. [32, 33] can account for the striking ADMR found in LTP of  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub>. Very similar ADMR has been seen also in M=Rb and Tl compounds. Therefore we conclude that LTP in  $\alpha$ -(BEDT-TTF)<sub>2</sub>MHg(SCN)<sub>4</sub> should be UCDW. Also we believe that ADMR provides clear signature for the presence of UCDW or USDW.

Before closing this section, we note that very similar ADMR has been seen in

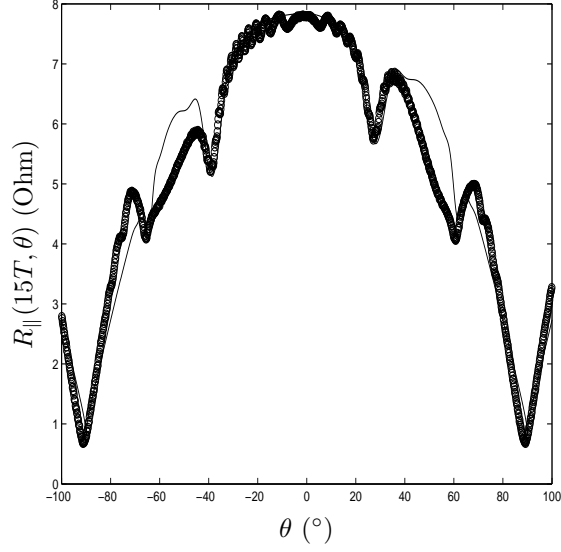


Fig. 7. The angular dependent magnetoresistance is shown for current parallel to the a-c plane at  $T = 1.4\text{K}$ ,  $B = 15\text{T}$ . The open circles belong to the experimental data, the solid line is our fit based on Eq. (25).

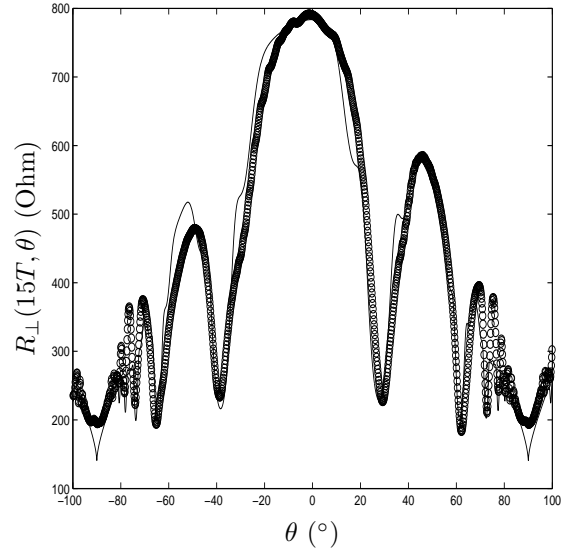


Fig. 8. The angular dependent magnetoresistance is shown for current perpendicular to the a-c plane at  $T = 1.4\text{K}$ ,  $B = 15\text{T}$ . The open circles belong to the experimental data, the solid line is our fit from Eq. (25).

Bechgaard salts  $(\text{TMTSF})_2\text{X}$  with  $\text{X}=\text{ClO}_4$ ,  $\text{PF}_6$  and  $\text{ReO}_4$ , when the magnetic field is rotated within the  $c^* - b$  plane [61–65]. In particular, ADMR in  $\text{PF}_6$  and

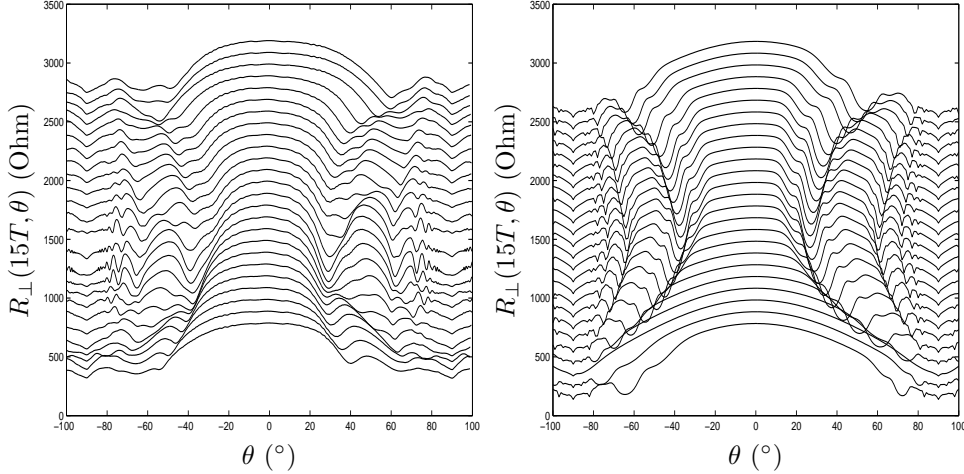


Fig. 9. ADMR is shown for current perpendicular to the a-c plane at  $T = 1.4\text{K}$  and  $B = 15\text{T}$  for  $\phi = -77^\circ, -70^\circ, -62.5^\circ, -55^\circ, -47^\circ, -39^\circ, -30.5^\circ, -22^\circ, -14^\circ, -6^\circ, 2^\circ, 10^\circ, 23^\circ, 33^\circ, 41^\circ, 48.5^\circ, 56^\circ, 61^\circ, 64^\circ, 67^\circ, 73^\circ, 80^\circ, 88.5^\circ, 92^\circ$  and  $96^\circ$  from bottom to top. The left (right) panel shows experimental (theoretical) curves, which are shifted from their original position along the vertical axis by  $n \times 100\text{Ohm}$ ,  $n = 0$  for  $\phi = -77^\circ$ ,  $n = 1$  for  $\phi = -70^\circ, \dots$

$\text{ReO}_4$  compounds are very close to ADMR that we discussed so far. It is known that this striking angular dependence is seen only in the "normal state". This means that conventional SDW and superconductivity has to be destroyed by pressure and magnetic field, respectively. Also the magnetic field has to be less than the one which produces the field induced SDW [4]. Also the dips are called Lebed resonances [66,67], but the shape of ADMR has not been understood. Indeed, USDW in this  $P - B$  phase diagram will describe this mysterious ADMR very consistently [68]. We have suggested earlier, that USDW appears in  $(\text{TMTSF})_2\text{PF}_6$  in addition to conventional SDW for  $T < T_c/3$ , where  $T_c$  is the transition temperature of SDW for  $p < 7$  kbar [69]. Therefore the presence of USDW in a large area of the  $P - B$  phase diagram may not be so surprising.

### 5. Seebeck and Nernst effect

The analysis in the preceding section is readily extended to the magnetothermopower tensor [36]. First let us consider the diagonal magneto-thermoelectric power. This is given by

$$\begin{aligned}
 S(B, \theta, \phi) = & -\frac{R(B, \theta, \phi)k_B}{e} [\sigma_0 \zeta_0 + \\
 & + \sigma_1 \left( \zeta_0 \frac{\exp(-x_1) + \cosh(\zeta_0)}{\cosh(x_1) + \cosh(\zeta_0)} + \zeta_1 \frac{\exp(-x_1) + \cosh(\zeta_1)}{\cosh(x_1) + \cosh(\zeta_1)} + \right. \\
 & \left. + x_1 \left( \frac{\sinh(\zeta_0)}{\cosh(x_1) + \cosh(\zeta_0)} + \frac{\sinh(\zeta_1)}{\cosh(x_1) + \cosh(\zeta_1)} \right) \right) ] \quad (26)
 \end{aligned}$$

where  $x_1$ ,  $\zeta_0$  and  $\zeta_1$  have been defined after Eq. (25). In the thermoelectric power at low temperatures, the particle-hole symmetry breaking plays the crucial role. This means  $S \sim \sigma_0$ ,  $\sigma_1$ . In this treatment we have neglected the terms coming from  $\partial\sigma/\partial\mu$ , where  $\mu$  is the chemical potential. For example in many heavy fermion systems, where the Kondo effect is apparent, the terms arising from  $\partial\sigma/\partial\mu$  may be dominant. In this case we have

$$S^K(B, \theta, \phi) = \frac{\pi^2 k_B^2 T}{3e} R(B, \theta, \phi) \times \left[ 2 \frac{\partial\sigma_1}{\partial\mu} \left( \frac{\exp(-x_1) + \cosh(\zeta_0)}{\cosh(x_1) + \cosh(\zeta_0)} + \frac{\exp(-x_1) + \cosh(\zeta_1)}{\cosh(x_1) + \cosh(\zeta_1)} \right) + \frac{\partial\sigma_2}{\partial\mu} \right]. \quad (27)$$

So in the most general case, these terms have to be added together.

The Nernst effect is the off diagonal component of the thermoelectric power in the presence of magnetic field. Also its formulation is different from above. We have seen already that quasiparticle in UDW orbits around the magnetic field. Then when an electric field  $\mathbf{E}$  is applied within the conducting plane, the quasiparticle drifts with drift velocity  $\mathbf{v}_D$  perpendicular to both  $\mathbf{B}$  and  $\mathbf{E}$  ( $\mathbf{v}_D = (\mathbf{E} \times \mathbf{B})/B^2$ ). Then the heat current parallel to  $\mathbf{v}_D$  is given by  $\mathbf{J}_h = TS\mathbf{v}_D$ , where  $S$  is the entropy associated with the circling quasiparticles

$$S = eB \sum_n [\ln(1 + \exp(-\beta E_n)) + \beta E_n (1 + \exp(\beta E_n))^{-1}], \quad (28)$$

the sum over  $E_n$  has to be taken over all the Landau levels, and the magnetic field is assumed to be perpendicular to the  $a-c$  plane ( $\theta = 0^\circ$ ). Also for simplicity we have neglected the imperfect nesting terms. Then for small  $T$  and large  $B$ , Eq. (28) is well approximated by taking the  $n = 0$  and  $n = 1$  Landau levels. This gives

$$S = 2eB \left[ \ln(2) + 2 \ln \left( 2 \cosh \left( \frac{x_1}{2} \right) \right) - x_1 \tanh \left( \frac{x_1}{2} \right) \right]. \quad (29)$$

So the Nernst coefficient in this configuration can be calculated, after considering the effect of the two dimensional parts of the Fermi surface:

$$S_{xy} = -\frac{S}{B\sigma} = \frac{1}{\sigma} \left[ \frac{L_{2D}}{1 + \gamma^2 B^2} - 2e \left( \ln(2) + 2 \ln \left( 2 \cosh \left( \frac{x_1}{2} \right) \right) - x_1 \tanh \left( \frac{x_1}{2} \right) \right) \right], \quad (30)$$

where  $\sigma = 1/R = 4\sigma_1/(\exp(x_1) + 1) + \sigma_2$  from Eq. (25),  $L_{2D}$  stems from the two dimensional cylinders of the Fermi surface,  $\gamma = e\tau/m$ ,  $\tau$  is the field-free relaxation time,  $m$  is the effective mass of the electron. Again  $\sigma_1$  is related to the  $n = 1$  Landau level and  $\sigma_2$  contains the contribution from the  $n = 0$  Landau levels as well as from the elliptical Fermi surface. Recently both the magneto-thermoelectric power and the Nernst effect of LTP in single crystal  $\alpha$ -(BEDT-TTF)<sub>2</sub>KHg(SCN)<sub>4</sub> has been reported [37]. We show in Figs. 10, 11 and 12 the fitting of the experimental data with the theoretical expressions Eqs. (26) and (30). In these fittings again, we used  $\Delta \sim 17$  K,  $v_a \sim 10^6$  cm/s and  $\Delta(T)/\Delta(0) = \sqrt{1 - (T/T_c)^3}$ . Both the Seebeck

coefficient and the large negative Nernst effect are very consistently described in terms of UCDW [36].

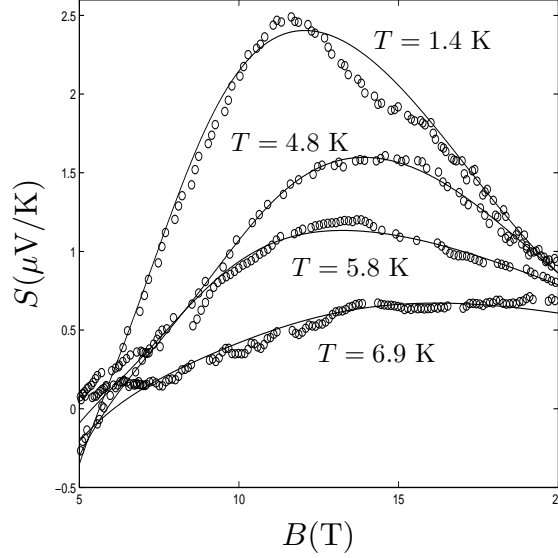


Fig. 10. The magnetothermopower for heat current along the  $a$  direction is shown for  $T = 1.4$  K,  $T = 4.8$  K,  $T = 5.8$  K and  $T = 6.9$  K from top to bottom, the circles denote the experimental data from Ref. [37], the solid line is our fit based on Eq. (26)

As already mentioned, the large negative Nernst signal has been reported in the underdoped region of LSCO, YBCO and Bi2212 [43–45]. A preliminary analysis indicated that the field dependence of this large Nernst effect can be described in terms of UDW [46]. Also it is well known that there are similarities between the 115 compounds  $\text{CeCoIn}_5$  and high  $T_c$  cuprate superconductors [70–73]. These are quasi-two dimensionality,  $d_{x^2-y^2}$ -wave superconductivity and the proximity to antiferromagnetism. More recently a large negative Nernst effect was observed above the superconducting transition temperature  $T_c = 2.3$  K [74]. We believe that this indicates UDW above superconductivity in  $\text{CeCoIn}_5$ .

## 6. Concluding remarks

We have reviewed recent theoretical advances in understanding the physics of UDW (i.e. UCDW and USDW). This was in part stimulated by the recent identification of the pseudogap phase of high  $T_c$  cuprates as d-wave density wave (d-DW), and in part by the identification of LTP in  $\alpha\text{-(BEDT-TTF)}_2\text{KHg(SCN)}_4$  as UCDW [75].

In particular in the latter case, the Landau quantization of the quasiparticle spectrum as discussed by Nersisyan et al. [32, 33] has played the crucial role. We propose here that both the striking angular dependent magnetoresistance (ADMR)

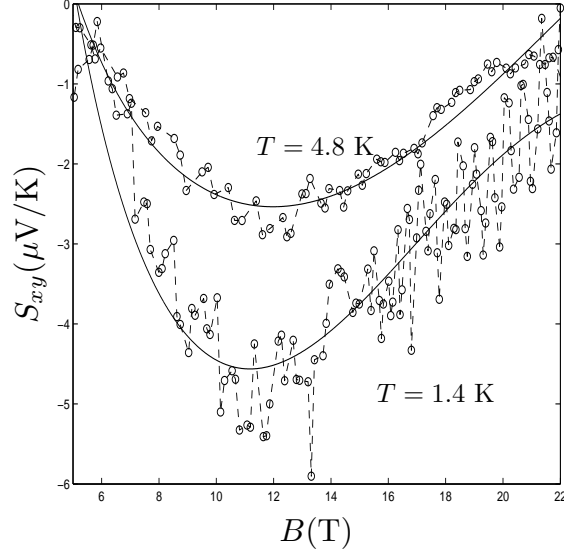


Fig. 11. The Nernst signal for heat current along the  $a$  direction is shown for  $T = 1.4$  K and  $T = 4.8$  K (from bottom to top), the dashed lines with circles denote the experimental data from Ref. [37], the solid line is our fit based on Eq. (30).

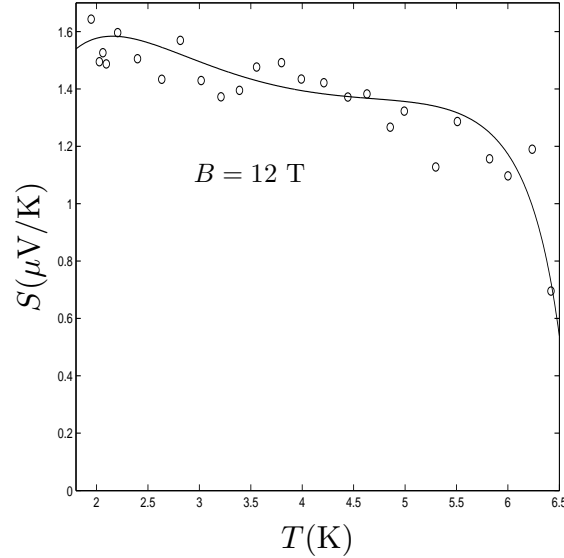


Fig. 12. The temperature dependence of the magnetothermopower for heat current along the  $a$  direction is shown for  $B = 12$  T, the circles denote the experimental data from Ref. [37], the solid line is our fit based on Eq. (26).

and the large negative Nernst signal provide the hallmark of UDW.

For example, the peculiar ADMR seen in Bechgaard salts  $(\text{TMTSF})_2\text{PF}_6$  and

(TMTSF)<sub>2</sub>ReO<sub>4</sub> in the limited  $P - B$  phase diagram suggests the presence of USDW in a wide region for  $T < 3$  K. Also UDW may inhabit many ground states in heavy fermion systems and organic conductors. In particular, the ground states in CeCoIn<sub>5</sub>, URu<sub>2</sub>Si<sub>2</sub>, CeCu<sub>2</sub>Si<sub>2</sub>,  $\kappa$ -(BEDT-TTF)<sub>2</sub>X with X=Cu(NCS)<sub>2</sub>, Cu[N(CN)<sub>2</sub>]Br, Cu[N(CN)<sub>2</sub>]Cl should be explored further [76–79]. Since the beginning of the 21st century, the gap symmetry of unconventional superconductors Sr<sub>2</sub>RuO<sub>4</sub>, CeCoIn<sub>5</sub>,  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>, YNi<sub>2</sub>B<sub>2</sub>C and PrOs<sub>4</sub>Sb have been determined. Likewise UDW becomes the density wave of the 21st century. In spite of very limited findings on this newly developing subject, we are confident that new discovery and new understanding of truly quantum condensates will modify and enrich our perspective on condensed matter physics in general. The vast forest with exotic birds and flowers are waiting for our exploration.

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### References

1. J. Sólyom, Adv. Phys. **28**, 201 (1979).
2. D. Jerome and H. Schulz, Adv. Phys. **31**, 299 (1982).
3. G. Grüner, *Density waves in solids* (Addison-Wesley, Reading, 1994).
4. T. Ishiguro, K. Yamaji, and G. Saito (Springer, Berlin, 1999).
5. J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
6. D. J. V. Harlingen, Rev. Mod. Phys. **67**, 515 (1995).
7. C. C. Tsuei and J. R. Kirtley, Rev. Mod. Phys. **72**, 969 (2000).
8. K. Maki and H. Won, Ann. Phys. (Leipzig) **5**, 320 (1996).
9. H. Won, Q. Yuan, P. Thalmeier, and K. Maki, Braz. J. Phys. **33**, 675 (2003).
10. B. I. Halperin and T. M. Rice, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic Press, New York, 1968), vol. 21, p. 115.
11. S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001).
12. A. Virosztek, K. Maki, and B. Dóra, Int. J. Mod. Phys. B **16**, 1667 (2002).
13. B. Dóra and A. Virosztek, Eur. Phys. J. B **22**, 167 (2001).
14. H. Won and K. Maki, Phys. Rev. B **49**, 1397 (1994).
15. L. Benfatto, S. Caprara, and C. Di Castro, Eur. Phys. J. B **17**, 95 (2000).
16. B. Dóra, A. Virosztek, and K. Maki, Acta Physica Polonica B **34**, 571 (2003).
17. T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999).
18. M. Oda, R. Kubota, K. Hoya, C. Manabe, N. Momono, T. Nakano, and M. Ido, Physica C **281**, 135 (1997).
19. T. Nakano, N. Momono, M. Oda, and M. Ido, J. Phys. Soc. Jpn **67**, 2622 (1998).



20. M. Kugler, O. Fischer, Ch. Renner, S. Ono, and Y. Ando, Phys. Rev. Lett. **86**, 4911 (2001).
21. J. Singleton, Rep. Prog. Phys. **63**, 1161 (2000).
22. P. Christ, W. Biberacher, M. V. Kartsovnik, E. Steep, E. Balthes, H. Weiss, and H. Müller, JETP Lett. **71**, 303 (2000).
23. D. Andres, M. V. Kartsovnik, W. Biberacher, H. Weiss, E. Balthes, H. Müller, and N. Kushch, Phys. Rev. B **64**, 161104(R) (2001).
24. M. Basletić, B. Korin-Hamzić, M. V. Kartsovnik, and H. Müller, Synth. Met. **120**, 1021 (2001).
25. see for example S. Tomić, J. R. Cooper, W. Kang, D. Jerome, and K. Maki, J. Phys. I (Paris) **1**, 1603 (1991).
26. B. Dóra, A. Virosztek, and K. Maki, Phys. Rev. B **64**, 041101(R) (2001).
27. B. Dóra, A. Virosztek, and K. Maki, Phys. Rev. B **65**, 155119 (2002).
28. T. Sasaki and N. Toyota, Phys. Rev. B **49**, 10120 (1994).
29. A. E. Kovalev, M. V. Kartsovnik, R. P. Shibaeva, L. P. Rozenberg, I. F. Schegolev, and N. D. Kushch, Solid State Commun. **89**, 575 (1994).
30. J. Caulfield, J. Singleton, P. T. J. Hendriks, J. A. A. J. Perenboom, F. L. Pratt, M. Doporto, W. Hayes, M. Kurmoo, and P. Day, J. Phys. Cond. Mat. **6**, L155 (1994).
31. N. Hanasaki, S. Kagoshima, N. Miura, and G. Saito, J. Phys. Soc. Japan **65**, 1010 (1996).
32. A. A. Nersesyan and G. E. Vachnadze, J. Low T. Phys. **77**, 293 (1989).
33. A. A. Nersesyan, G. I. Japaridze, and I. G. Kimeridze, J. Phys. Cond. Mat. **3**, 3353 (1991).
34. B. Dóra, K. Maki, B. Korin-Hamzić, M. Basletić, A. Virosztek, M. V. Kartsovnik, and H. Müller, Europhys. Lett. **60**, 737 (2002).
35. K. Maki, B. Dóra, M. Kartsovnik, A. Virosztek, B. Korin-Hamzić, and M. Basletić, Phys. Rev. Lett. **90**, 256402 (2003).
36. B. Dóra, K. Maki, A. Ványolos, and A. Virosztek, Phys. Rev. B **68**, 241102(R) (2003).
37. E. S. Choi, J. S. Brooks, and J. S. Qualls, Phys. Rev. B **65**, 205119 (2002).
38. M. Dressel, G. Grüner, J. P. Pouget, A. Breining, and D. Schweitzer, J. Phys. I France **4**, 579 (1994).
39. A. H. Castro-Neto, Phys. Rev. Lett. **86**, 4382 (2001).
40. H. Ikeda and Y. Ohashi, Phys. Rev. Lett. **81**, 3723 (1998).
41. R. Bel, K. Behnia, and H. Berger, Phys. Rev. Lett. **91**, 066602 (2003).
42. H. Amitsuka, M. Sato, N. Metoki, M. Yokoyama, K. Kuwahara, T. Sakakibara, H. Morimoto, S. Kawarazaki, Y. Miyako, and J. A. Mydosh, Phys. Rev. Lett. **83**, 5114 (1999).
43. C. Capan, K. Behnia, J. Hinderer, A. G. M. Jansen, W. Lang, C. Marcenat, C. Marin, and J. Flouquet, Phys. Rev. Lett. **88**, 056601 (2002).
44. Y. Wang, Z. A. Xu, T. Kakeshita, S. Uchida, S. Ono, Y. Ando, , and N. P. Ong, Phys. Rev. B **64**, 224519 (2001).
45. Y. Wang, N. P. Ong, Z. A. Xu, T. Kakeshita, S. Uchida, D. A. Bonn, R. Liang, , and W. N. Hardy, Phys. Rev. Lett. **88**, 257003 (2002).
46. K. Maki, B. Dóra, A. Ványolos, and A. Virosztek, Curr. Appl. Phys. (in press).
47. Y. Nambu, Phys. Rev. **117**, 648 (1960).
48. Y. Sun and K. Maki, Phys. Rev. B **51**, 6059 (1995).
49. T. Hotta, J. Phys. Soc. Jpn. **62**, 274 (1993).
50. Y. Sun and K. Maki, Europhys. Lett. **32**, 355 (1995).
51. B. Dóra, A. Virosztek, and K. Maki, Phys. Rev. B **66**, 115112 (2002).
52. B. Dóra, A. Virosztek, and K. Maki, Phys. Rev. B **68**, 075104 (2003).

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53. K. Yamaji, J. Phys. Soc. Japan **51**, 2787 (1982).
54. X. Huang and K. Maki, Phys. Rev. B **46**, 162 (1992).
55. L. D. Landau, Soviet Phys. JETP **3**, 920 (1957).
56. L. D. Landau, Soviet Phys. JETP **5**, 101 (1957).
57. L. D. Landau, Soviet Phys. JETP **8**, 70 (1959).
58. A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover Publications, New York, 1963).
59. W. Heisenberg and H. Euler, Z. Phys. **98**, 714 (1936).
60. V.S.Weisskopf, Kongelige Danske Videns. Selskab Matematisk-fsiske Meddelelser **6**, 14 (1936).
61. T. Osada, A. Kawasumi, S. Kagoshima, N. Miura, and G. Saito, Phys. Rev. Lett. **66**, 1525 (1991).
62. M. J. Naughton, O. H. Chung, M. Chaparala, X. Bu, and P. Coppens, Phys. Rev. Lett. **67**, 3712 (1991).
63. W. Kang, S. T. Hannahs, and P. M. Chaikin, Phys. Rev. Lett. **69**, 2827 (1992).
64. I. J. Lee and M. J. Naughton, Phys. Rev. B **58**, R13343 (1998).
65. W. Kang, H.-Y. Kang, Y. J. Jo, and S. Uji, Synth. Met. **133**, 15 (2003).
66. A. G. Lebed, JETP Lett. **43**, 174 (1986).
67. A. G. Lebed and P. Bak, Phys. Rev. Lett. **63**, 1315 (1989).
68. B. Dóra, K. Maki, and A. Virosztek, in preparation.
69. M. Basletić, B. Korin-Hamzić, and K. Maki, Phys. Rev. B **65**, 235117 (2002).
70. M. Nicklas, R. Borth, E. Lengyel, P. G. Pagliuso, J. L. Sarrao, V. A. Sidorov, G. Sparn, F. Steglich, and J. D. Thompson, J. Phys. Cond. Matt. **13**, L905 (2001).
71. K. Izawa, H. Yamaguchi, Y. Matsuda, H. Shishido, R. Settai, and Y. Onuki, Phys. Rev. Lett. **87**, 057002 (2001).
72. I. Shishido, R. Settai, D. Aoki, S. Ikeda, H. Nakawaki, N. Nakamura, T. Iizuka, Y. Inada, K. Sugiyama, T. Takeuchi, K. Kindo, T. C. Kobayashi, *et al.*, J. Phys. Soc. Jpn. **71**, 162 (2002).
73. V. A. Sidorov, M. Nicklas, P. G. Pagliuso, J. L. Sarrao, Y. Bang, A. V. Balatsky, and J. D. Thompson, Phys. Rev. Lett. **89**, 157004 (2003).
74. R. Bel, K. Behnia, Y. Nakajima, K. Izawa, Y. Matsuda, H. Shishido, R. Settai, and Y. Onuki, cond-mat/0311473.
75. K. Maki, B. Dóra, and A. Virosztek (AIP Conference Proceedings 695, Melville, 2003), p. 10.
76. K. Kanoda, Physica C **282-287**, 299 (1997).
77. K. Izawa, H. Yamaguchi, T. Sasaki, and Y. Matsuda, Phys. Rev. Lett. **88**, 027002 (2002).
78. J. Müller, M. Lang, F. Steglich, J. A. Schlueter, A. M. Kini, and T. Sasaki, Phys. Rev. B **65**, 144521 (2002).
79. M. Pinterić, S. Tomić, M. Prester, D. Dorbać, and K. Maki, Phys. Rev. B **66**, 174521 (2002).